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Pade spectroscopy of structural correlation functions: Application to liquid gallium

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Abstract

© 2016, Pleiades Publishing, Inc.We propose the new method of fluid structure investigation based on numerical analytic continuation of structural correlation functions with Pade approximants. The method particularly allows extracting hidden structural features of disordered condensed matter systems from experimental diffraction data. The method has been applied to investigate the local order of liquid gallium, which has a non-trivial structure in both the liquid and solid states. Processing the correlation functions obtained from molecular dynamic simulations, we show the method proposed reveals non-trivial structural features of liquid gallium such as the spectrum of length-scales and the existence of different types of local clusters in the liquid.

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